

**ANTIBACTERIAL ACTIVITY OF TERPENE NATURAL
COMPOUNDS FROM APOCYNACEAE AGAINST
KLEBSIELLA PNEUMONIAE: IN SILICO STUDY**

SAJIDA AM SABBAH



**PROGRAM STUDY OF MICROBIOLOGY
FACULTY OF MATHMATICS AND NATURAL SCIENCES
IPB UNIVERSITY
BOGOR
2024**

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Sajida AM Sabbah
G3501202802

SUMMARY

SAJIDA AM SABBAH. Antibacterial Activity of Terpene Natural Compounds against *Klebsiella pneumoniae*: *in silico* study. Supervised by RIKA INDRI ASTUTI and SRI BUDIARTI.

Klebsiella pneumoniae, a Gram-negative, nonmotile, encapsulated rod-shaped bacterium, has become an emerging nosocomial pathogen that can cause clinical infectious diseases. Through the years, frequent use and contact with antibiotics in hospitals have created antibiotic-resistant *K. pneumoniae* strains, limiting available treatment options for medical intervention against infections. Many proteins support the property of antibiotic resistance and one of these proteins found in *Klebsiella* bacteria is beta-lactamase SHV-1.

Many terpenes are known to be active against a wide variety of microorganisms, including gram-positive and gram-negative bacteria and fungi. Toxic effects on membrane structure and function have been generally used to explain the antimicrobial action of essential oils and their monoterpenoid components.

Monoterpene indole alkaloids (MIAs) are compounds that are identified from six genera of the Apocynaceae family. The following genera are *Alstonia*, *Rauvolfia*, *Kopsia*, *Ervatamia*, *Tabernaemontana*, and *Rhazya*. Traditionally, plant species of this family have been used for the treatment of fever, malaria, gastrointestinal ailments, diabetes, and pain. There are many terpenes natural compounds (>400 compounds). Thus, finding the terpene compounds that strongly interact with the targeted protein in *K. pneumoniae* would serve as a potential strategy to find the most potent compounds.

The recent study examined the potential interactions between beta-lactamase (bla-SHV-1), a protein that supports antibiotic resistance in *Klebsiella*, and MIAs from six genera of plants in the Apocynaceae family. The MIAs were used as ligands in this study. The PyRx program for molecular docking and other computer programs were used to assess the effectiveness of MIAs as inhibitors (PyMOL, LigPlot+, Discovery Studio, Notepad, Gimp 2.10).

In this study the initial molecular docking investigation identified several MIAs with potential as inhibitors. Paucidisine, (-)-19-Oxoisoeburnamine, and paucidactine A demonstrated the most promise. Ligand-protein interactions, such as hydrogen bonds and hydrophobic interactions, were also analysed to determine the best terpenes. The most effective terpenes showed a higher percentage of similarity when compared to native ligands.

It is important to note that these findings are based on an *in silico* study and require *in vitro* confirmation before being considered for future drug design. Overall, this study takes a significant step towards discovering alternative treatment options for antibiotic-resistant *Klebsiella* infections. By exploring the potential of MIAs as inhibitors, this research offers a promising avenue for combating antibiotic resistance and improving patient outcomes.

Keywords: *Klebsiella pneumoniae*, Antibiotic-resistant, Beta-lactamase, *In silico*, Monoterpene Indole Alkaloids



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SAJIDA AM SABBAH

**Thesis
as one of the requirements to obtain the
Master degree on
Microbiology Study Program**

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External Examiner of Thesis Examination:

- 1 Dr. Setyanto Tri Wahyudi, M.Si.

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Thesis Title: Antibacterial Activity of Terpene Natural Compounds From Apocynaceae
against *Klebsiella pneumoniae*: *in silico* study

Name : Sajida A.M Sabbah
NIM : G3501202802

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Approved by

Main Supervisor:
Dr. Rika Indri Astuti, S.Si, M.Si



Co-Supervisor:
Prof.Dr. Sri Budiarti



Agreed by

Head of Microbiology Study Program:
Prof. Dr. Dra. Anja Meryandini, M.S
NIP 19620327 198703 2 001



Vice Dean of Academic and Student Affairs:
Dr. Berry Juliandi, S.Si., M.Si
NIP 198008232007011001



Date of The Examination: 6 June 2024

Date of Graduation:

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Praise Allah SWT who has bestowed His grace, guidance, and gifts, so the Research Proposal entitled Antibacterial Activity of Terpene Natural Compounds against *Klebsiella pneumoniae*: *in silico* study has been completed. The research will be carried out from January 2022 and will be completed in July 2023. The author took the theme to predict the most active terpene compound by docking and its antimicrobial activity against *K. pneumoniae*. This research is compiled as a prerequisite for obtaining a Master of Science degree in the Microbiology Study Program, at Bogor Agricultural University.

I would like to thank Dr. Rika Indri Astuti MSi and Prof.Dr. Sri Budiarti is the supervisor commission in this research. Thank you to Prof. Dr. Anja Meryandini, MS the Head of the Microbiology Study Program, all staff of the Department of Biology, and all those who have helped in completing this research.

The author hopes that this research can serve as a guide in the thesis research and be useful for readers, especially those interested in microbiology. The author realizes that in the preparation and writing of this research there are still many shortcomings, so the author hopes for suggestions. Hopefully, this research can be useful for those who read it.

Bogor, June 2024

Sajida AM Sabbah

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